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Electric field induced shifts in electronic states in spherical quantum dots with parabolic confinement

C Bose
Department of Electronics and Telecommunication Engineering, Jadavpur University, Calcutta-700 032, India
and
C K Sarkar
Department of Physics, B E College, Deemed University, Shibpur, Howrah-711 103, India

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Abstract : An attempt is made to investigate the electric field induced shifts in electronic states in a spherical quantum dot (QD) with an isotropic parabolic potential (PP) The perturbation method is used to estimate the shifts of the above energy levels due to an uniform electric field. The energy shift of the lowest state is also worked out by the variational method, and compared with the results obtained from the perturbation method Both the methods are found to yield exactly identical results within the range of the applied field considered In the case of a spherical QD with square-well potential (SWP), the ground level shift is also compared with the above results

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Studies of nanostructured semiconductors exhibiting quantum confinement in all three dimensions have been made possible by the recent progress in nanoscale lithography and microcrystallite doping of glasses. Research on electro-optic effects in such quasi-zero-dimensional (QOD) systems is attracting increasing attention, due to their applicability in the field of optoelectronics [1,2]. The electric field-induced shifts in excitonic and electronic energy levels have already been investigated for a spherical QD with SWP [3,4]. A number of both theoretical and experimental works, however, indicate that the in-plane confinement in QDs is approximately parabolic [5,6]. These observations have stimulated further interest in QDs with parabolic confining potential [7]. In this communication, we shall investigate the effect of electric field on electronic states of such QDs. We shall first derive an expression for the shifts in electronic energy levels, due to the field applied on a spherical parabolic QD made of a typical wide-gap semiconductor, by using the perturbation method. The field-induced shift in the ground level of the above system will also be derived by the variational method, and the results will be compared with that obtained by the perturbation method. Similar results for a spherical QD with SWP will also be compared with the above results. Since GaAs is a typical example of wide-gap semiconductors, we will consider GaAs QDs to compute the energy level shifts.

In order to estimate the Stark shift of electronic energy levels in a spherical QD with isotropic parabolic potential, we assume the barrier height to be infinite for simplicity. In absence of electric field, the wavefunction of electrons confined within a spherical QD, can be expressed in polar coordinate as

$$\psi_{nlm} = R_{nl}(r) Y_{lm}(\theta, \phi), \tag{1}$$

where $Y_{lm}(\theta,\phi)$ is the angle dependent part and $R_{nl}(r)$ is the radial part, which in its normalized form can be given by [8]

$$R_{nl}(r) = \sqrt{\frac{2n!}{\Gamma(n+l+3/2)}} \beta^{(l+3/2)/2} r^l \exp(-\beta r^2/2) L_n^{(l+1/2)}(\beta r^2). \tag{2}$$

In the above equation, $\beta = m^* \omega / \hbar, \hbar = \frac{h}{2\pi}$, where h is Planck's constant, m^* is effective mass of electron, ω is the parabola frequency, L_n^α is Laugurre Polynomial of order n and degree α, Γ is Gamma function, n (= 0, 1, 2, 3, ...) is the principal quantum number, l (= 0, 1, 2, 3, .. .) is the angular momentum quantum number, and m (= 0, ±1, ±2, . . , ±l) is the magnetic quantum number. The corresponding energy eigenvalue E_{nlm} is given by

$$E_{nlm} = (2n + l + 3/2) \hbar \omega. \tag{3}$$

Let us assume that an uniform electric field F_e be applied in the polar direction (*i.e.* z-direction). For electric fields higher than 10^7 V/m, the voltage drop across the dot may be comparable to the barrier height, making the assumption of infinite barrier QD no longer valid. We therefore, restrict the magnitude of the applied field to the value 10^6 V/m in the present analysis.

In the presence of the electric field F_e, the Hamiltonian of the system takes the form

$$H = \frac{p^2}{2m^*} + \frac{1}{2} m^* \omega^2 r^2 + eFr\cos\theta, \tag{4}$$

where e is the electronic charge, p is the momentum, θ is the polar angle and F is the field inside the QD. The field F is, however, related to the external field F_e by the familiar expression

$$3\varepsilon_e \tag{5}$$

where ε_d and ε_e are the dielectric constants of the QD and the embedding material respectively.

The energy levels of electrons confined in the spherical QD get shifted due to the applied field and such shifts are derived separately by using the perturbation and the variational methods.

The perturbation method :

For the range of electric field considered here, the effect of the field can be treated as a small perturbation over the original Hamiltonian. The energy levels in the presence of a field, can be corrected to the second order in F, by applying the standard perturbation technique. The first order correction term vanishes due to the orthogonal property of spherical harmonics. The second order correction term, giving the shifts in the energy levels due to the applied field, can finally be obtained as

$$\Delta E_{nlm} = \sum_{n'} \frac{|b_{l,m} I_1|^2}{E_{n,l,m} - E_{n',l+1,m}} + \sum_{n'} \frac{|b_{l-1,m} I_2|^2}{E_{n,l,m} - E_{n',l-1,m}}, \tag{6}$$

where $$I_1 = eF\left[\frac{n!n'!}{\beta\Gamma(n+l+3/2)\Gamma(n'+l+5/2)}\right]^{1/2} I_1', \tag{7}$$

$$I_2 = eF\left[\frac{n!n'!}{\beta\Gamma(n+l+3/2)\Gamma(n'+l+1/2)}\right]^{1/2} I_2' \tag{8}$$

with $$I_1' = \int_0^\infty x^{l+3/2}\exp(-x)L_n^{l+1/2}(x)L_{n'}^{l+3/2}(x)dx, \tag{9}$$

and $$I_2' = \int_0^\infty x^{l+1/2}\exp(-x)L_n^{l+1/2}(x)L_{n'}^{l-1/2}(x)dx \tag{10}$$

and $$b_{lm} = \left[\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}\right]^{1/2}. \tag{11}$$

The variational method :

To perform the variational calculation, the ground state trial wavefunction for electrons in the presence of electric field, is taken as

$$\psi = N(\lambda)\exp(-\beta r^2/2)\exp(-\lambda r\cos\theta), \tag{12}$$

where λ is the variational parameter and $N(\lambda)$ is the normalisation constant, given by

$$N(\lambda) = (\beta/\pi)^{3/4}\exp\left(\frac{\lambda^2}{2\beta}\right). \tag{13}$$

The corresponding energy eigenvalue is

$$E(\lambda) = \frac{\hbar^2}{2m^*}\left[\lambda^2 - \frac{2\lambda m^* eF}{\beta\hbar^2} + 3\beta\right. \tag{14}$$

where $\lambda = \frac{eF}{\hbar\omega}$. With this value of λ, the shift in the ground level energy (E_0) induced by the applied field, is given as

$$\Delta E_0 = -\frac{e^2F^2}{2m^*\omega^2} \tag{15}$$

To find the effect of parabolic confinement, we compare the field induced shifts in the ground state energy, as calculated above, with that of an identical spherical QD having SWP. To estimate the ground level shift in the latter case, we use the relation derived by Nomura and Kobayashi [9], using variational technique. According to their derivation the energy shift is given by

$$\Delta E_0 = -\frac{(2\pi^2-3)^2}{108\pi^2}E_0\phi^2, \tag{16}$$

where $\phi = \frac{eFR}{E_0}$, R being the radius of the spherical dot.

Field induced energy level shifts in spherical QD with parabolic confinement have been computed by taking material parameters for GaAs [10]. The energy shifts have been calculated for the ground state by the perturbation as well as by the variational methods. The computed results have been tabulated in Table 1. It can be seen from the table that the two methods give identical results.

Table 1. Energy shift (ΔE) of the ground state electron in GaAs spherical parabolic QD, obtained using the second order perturbation method and the variational method.

Field (V/m)	β (nm^{-2})	$\Delta E_{\text{perturbation}}$ (meV)	$\Delta E_{\text{variational}}$ (meV)
	3.28987×10^{18}	-4.05876×10^{-7}	-4.05877×10^{-7}
1×10^5	1.31595×10^{17}	-2.53672×10^{-4}	-2.53673×10^{-4}
	3.28987×10^{16}	-4.05876×10^{-3}	-4.05877×10^{-3}
	3.28987×10^{18}	-1.01469×10^{-5}	-1.01469×10^{-5}
5×10^5	1.31595×10^{17}	-6.34181×10^{-3}	6.34182×10^{-3}
	3.28987×10^{16}	-0.101469	0.101469
	3.28987×10^{18}	-4.05876×10^{-5}	-4.05877×10^{-5}
$\times 10^6$	1.31595×10^{17}	-0.0253672	-0.0253673
	3.28987×10^{16}	-0.405876	-0.405877

The shift in the ground level energy as a function of applied field is shown in Figure 1, both for QD with SWP and QD with PP. The energy reference point in this figure is chosen at zero field. To compare the shift in energy level in the two systems, the ground state energies of both the structures have been taken to be equal. Here, we note that the energy in QD with PP is $\sim \hbar\omega = \frac{\hbar^2\beta}{m^*}$. The parameter β, therefore, scales as $\frac{1}{R^2}$ (*i.e.* $R \sim \beta^{-1/2}$). The parameters in Figure 1 have, therefore, been chosen as dot radius R for QD with SWP and $\beta^{-1/2}$ for QD with PP. Figure 1 shows an increase in energy shift with increase in applied field. This can be ascribed to the enhanced overlap between adjacent

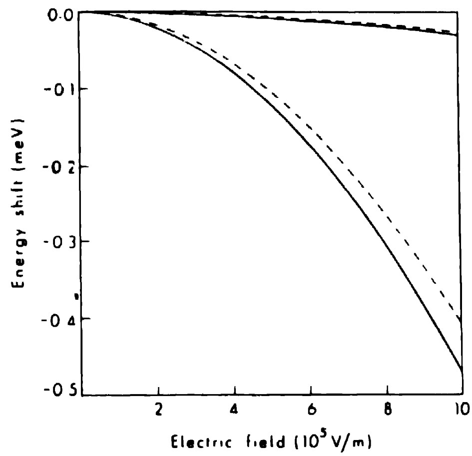

Figure 1. A comparison of the electron ground-state energy shift as obtained from the spherical QD with SWP (solid line) and PP (broken line). The upper and the lower set of curves are for dots of radius R = 5 nm and 10 nm respectively. The results are calculated from a variational treatment.

wavefunctions with increase in electric field. It is also seen from the figure that the shift in the lowest energy level in spherical dot with SWP, calculated by the variational method, is more than that in QD with PP. The adjacent higher-lying levels are closer to the ground level in the QD with SWP as compared to the QD with PP. This leads to more pronounced field induced shift in the case of SWP. Energy shifts have also been computed for few higher-lying levels of a spherical dot with PP. The shifts, which have been found to be the same for all levels, are due to equal interlevel energy separation.

Figure 2 presents the variation of the ground level shift in a QD with parabolic confinement as a function of the parameter $\beta^{-1/2}$ *i.e.*, effectively of the dot size, for three different electric fields. Here, the energy reference point has been chosen at $\beta^{-1/2}$ = 0.55 nm, which corresponds to the smallest spherical dot (with SWP) of 1 nm radius. From the figure, it can be seen that the energy shift increases with increase in the value of $\beta^{-1/2}$ *i.e.*, of the physical dimension of the dot, as expected. The more prominent variations are observed for larger field strengths.

To sum up, the effect of the parabolic confinement is seen to reduce the field induced shift in the lowest energy state of a spherical QD, as compared to a dot with SWP. In addition, the parabolic confinement makes the lowering of different levels insensitive to level energies. The perturbation and the variational methods, employed to estimate the ground level energy shift, yield identical results while being computed for a spherical QD with PP.

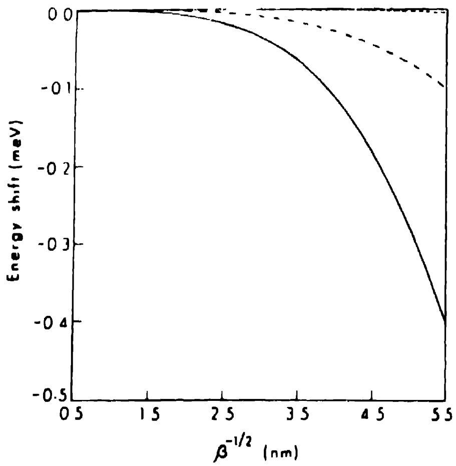

Figure 2. Energy shifts of the ground state electron in a GaAs spherical QD with parabolic confinement as a function of $\beta^{-1/2}$ for three representative electric fields of $F = 1 \times 10^6$ V/m (solid line), 5×10^5 V/m (dashed line) and 1×10^5 V/m (dotted line)

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